

Summary--Quantum Physics Units 10, 11 and 12

We learned that we can extend a lot of our notions of waves to the behavior of microscopic objects, especially sub-atomic particles like electrons, protons, and neutrons, through the relationship first proposed by Louis DeBroglie

$$p = \frac{h}{\lambda}, \text{ where}$$

$$h = 6.626 \times 10^{-34} \text{ J sec.}$$

The whole notion of representing a particle by a wave function is a little bizarre. We tried to patch this up by making the waves into wave packets, but found that as we localized them more and more, the wave character disappeared. We argued that this became critical when the packet width was comparable to the wavelength, then our uncertainty became comparable to the value itself, so it is plausible that the combination of this uncertainty with the DeBroglie relation gives the Heisenberg uncertainty principle

$$\Delta_s p \Delta_s x > h/4\pi$$

where the subscript s reminds us that the Δ is defined to be the standard deviation of the spread of values of x or p. More commonly, we use the Δ to refer to a complete range, as for a particle confined between two walls, in which case we gain roughly a factor of 3 over the standard deviation, and here, it is more appropriate to make the approximation

$$\Delta p \Delta x > h.$$

We did not even demonstrate this in any generality, let alone prove it, although it is not terribly difficult to do so. This principle tells us that if we attempt to confine a particle to a small region, this forces us to accept an uncertainty in the momentum. In other words, if we were to prepare a set of identical systems consisting of a confined particle, and then measure the momentum of the particle, no matter how much we tried to make the momentum zero, we would get a variety of measured values spread out randomly with a range of at least Δp .

We then proceeded to develop a graphic analogy for quantum waves. These waves have two degrees of freedom that are usually represented by a complex (real and imaginary parts) wave; we represent them by colors, or hues, and brightness in a picture. The rules for quantum evolution say that the wave evolves by "rotating" through the color spectrum, keeping the intensity constant. [In fact, this rule is true only for the set of quantum waves that have well-defined energies, which are the wave functions chemists and physicists normally consider.] Given this rule, a moving particle is described by a rainbow of colors in a line, where the order of the colors determines which direction the wave/particle is traveling. As with classical waves, we can superpose two waves traveling in opposite directions and produce standing waves. Just as classical standing waves were useful for describing the vibrations confined by boundaries at either end, like a vibrating string on a musical instrument, these quantum standing waves allow us to describe the allowed states of a particle confined to a one-dimensional region, the so-

called particle in a box. Using the fact that the kinetic energy can be related to the momentum by

$$E = p^2/2m$$

we find that the allowed energies are

$$E = \frac{n^2 h^2}{8mL^2}$$

where L is the length of the region, and n is an integer that describes the number of half wavelengths in the region: 1, 2, 3, etc.

Quantum mechanics says that only these "quantized" energies are allowed, so that changes in energy must be accompanied by a sudden emission or absorption of energy, often in the form of a photon of light, with an energy that is equal to the difference between the energies of the two quantum "levels."

Finally we also looked at waves confined to a circular region, and found that they were also quantized. They gave rise to energies of

$$E = \frac{n^2 h^2}{8m\pi^2 r^2}$$

and the quantization of the angular momentum in units of $h / 2\pi \equiv \hbar$:

$$L = \frac{nh}{2\pi} = n\hbar.$$

We moved on to the investigation of quantum mechanics in multiple dimensions by considering particles confined to a box. Here we again were fitting standing waves, only now in multiple dimensions, which gave us the allowed energy values

$$E = \frac{h^2}{8m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right).$$

For the hydrogen atom, we have a system with spherical symmetry, so we need to imagine wrapping waves around the nucleus in a way that acknowledges this symmetry. We create now nodal surfaces rather than points, as in one dimension, or lines, as in two dimensions. These nodes can exist in the radial (r) direction, where they are spherical surfaces, or in the θ direction, where they form cones (or the degenerate cone which is the equatorial plane), or in the ϕ direction. For this latter case, since ϕ wraps around on itself, the waves in this direction can actually go through the color spectrum, as long as it comes back to the same color after one pass around. In this case, the number of times the color spectrum is traversed in one trip around ϕ is the number of nodes in this direction. So, in each of these directions, we may choose an arbitrary number of nodes, starting at zero. We labeled these with the quantum numbers n_r , n_θ , and n_ϕ . This notation is our own, however, the conventional notation is n , ℓ , and m_ℓ . The relationship between our quantum numbers and the conventional notation is as follows:

$$n = n_r + n_\theta + |n_\phi| + 1$$

$$\ell = n_\theta + |n_\phi|$$

$$m_\ell = n_\phi$$

which then makes the restrictions $\ell < n$ and $-\ell \leq m_\ell \leq \ell$ obvious. Why these new quantum numbers, you might ask? The answer lies in the observable quantities of energy and angular momentum, where

$$E = -\frac{2.2 \times 10^{-18} \text{ J}}{n^2}$$

$$L^2 = \frac{\ell(\ell+1)\hbar^2}{(2\pi)^2} = \ell(\ell+1)\hbar^2$$

$$L_z = \frac{m_\ell \hbar}{2\pi} = m_\ell \hbar$$

When we add more than one electron to an atom, we make the approximation that each electron fits into a hydrogen-like quantum state. This is affected by the existence of spin (a new quantum variable, an intrinsic angular momentum of the electron, that is allowed to have two possible values, which we call up and down) and the Pauli Exclusion Principle, which forbids any two electrons to have exactly the same quantum numbers. We put electrons in the lowest possible levels, and the number of combinations we can find give us 2 electrons in the $n = 1$ level, 8 electrons in the $n = 2$ level, and so on. Particularly stable atoms result when an n level is filled, particularly reactive atoms when the structure has only one electron more or less than a filled shell.